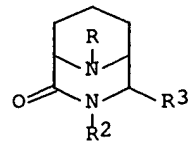
L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2001 ACS
AN 2000:68456 CAPLUS
DN 132:107945
TI Preparation of 9-trimethoxyphenyloxalyl-2-oxo-3,9-diaza[3.3.1]nonanes and analogs as FKBP rotamase inhibitors
IN Katoh, Susumu; Kawakami, Hiroshi; Tada, Hiroki; Linton, Maria Angelica; Kalish, Vincent; Tatlock, John Howard; Villafranca, J. Ernest
PA Agouron Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000004020	A1	20000127	WO 1999-US15965	19990715
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9949963	A1	20000207	AU 1999-49963	19990715
PRAI	US 1998-93299		19980717		
	US 1999-132884		19990506		
	WO 1999-US15965		19990715		

OS MARPAT 132:107945
GI



I

AB Title compds. [I; R = COCOR1; R1 = H, (cyclo)alk(en)yl, aryl, etc.; R2 = H, (ar)alkyl, alkoxy(alkyl), alkanoyloxy(alkyl), etc.; R3 = H, cyano, alkoxy, etc.; R2R3 = atoms to complete a ring] were prepd. Thus, piperidine-2,6-dicarboxylic acid was N-protected and the product treated with Ac2O to give the anhydride which was cyclocondensed with PhCH2OCH2CH2NH2 to give, in 3 addnl. steps, I (R2 = CH2CH2OCH2Ph, R3 = H)(II; R = H) which was N-acylated by 3,4,5-(MeO)3C6H2COCO2H to give II [R = COCOC6H2(OMe)3-3,4,5]. Data for biol. activity of I were given.

IT **255909-35-4P 255909-38-7P 255909-39-8P**
255909-41-2P 255909-42-3P 255909-43-4P
255909-44-5P 255909-45-6P 255909-46-7P
255909-48-9P 255909-53-6P 255909-57-0P
255909-59-2P 255909-60-5P 255909-65-0P
255909-66-1P 255909-67-2P 255909-68-3P
255909-69-4P 255909-70-7P 255909-72-9P
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255909-76-3P 255909-77-4P 255909-82-1P
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255910-06-6P 255910-07-7P 255910-10-2P
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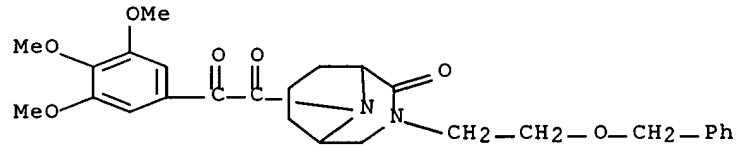
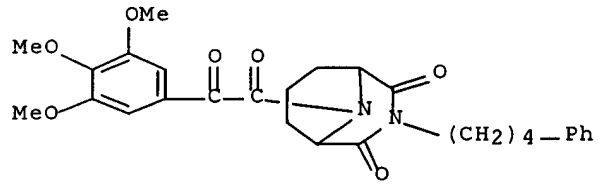
255910-14-6P 255910-15-7P 255910-20-4P
255910-21-5P 255910-22-6P 255910-23-7P
255910-24-8P 255910-32-8P 255910-50-0P
255910-51-1P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 9-trimethoxyphenyloxalyl-2-oxo-3,9-diaza[3.3.1]nonanes and analogs as FKBP rotamase inhibitors)

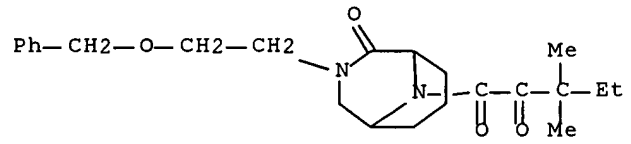
RN 255909-35-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-[2-(phenylmethoxy)ethyl]- (9CI) (CA INDEX NAME)



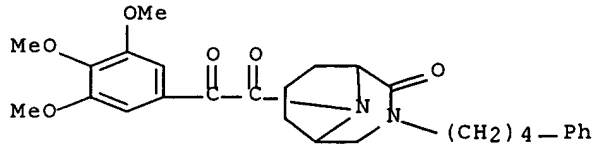
RN 255909-38-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



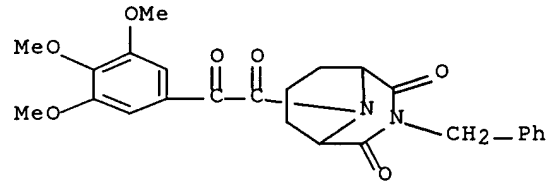
RN 255909-39-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-[2-(phenylmethoxy)ethyl]- (9CI) (CA INDEX NAME)



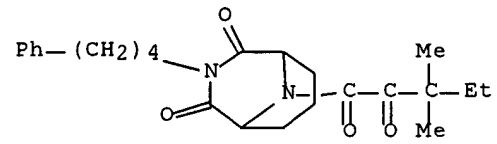
RN 255909-41-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



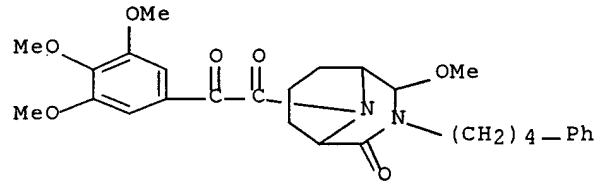
RN 255909-42-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



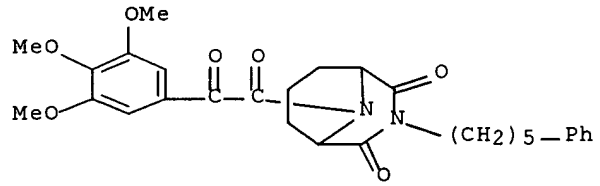
RN 255909-43-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



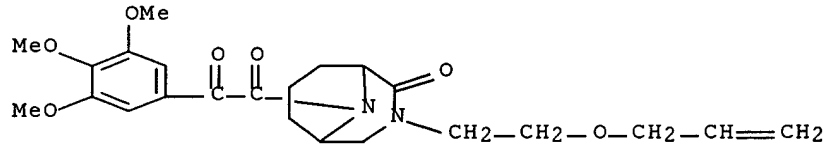
RN 255909-44-5 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 4-methoxy-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



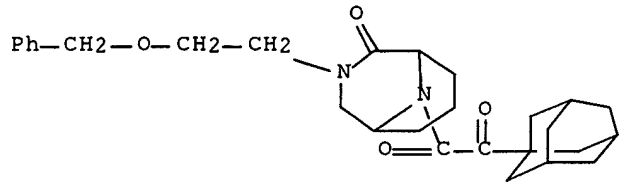
RN 255909-45-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(5-phenylpentyl)- (9CI) (CA INDEX NAME)



RN 255909-46-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-[2-(2-propenyloxy)ethyl]- (9CI) (CA INDEX NAME)

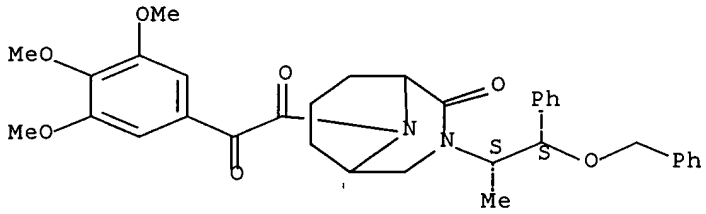


RN 255909-48-9 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(oxotricyclo[3.3.1.13,7]dec-1-ylacetyl)-3-[2-(phenylmethoxy)ethyl]- (9CI) (CA INDEX NAME)



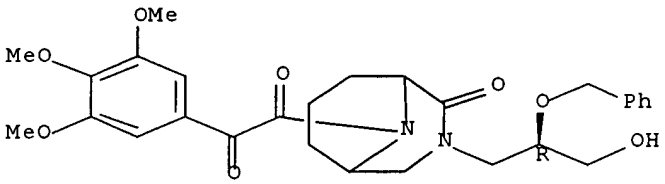
RN 255909-53-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[(1R,2R)-1-methyl-2-phenyl-2-(phenylmethoxy)ethyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



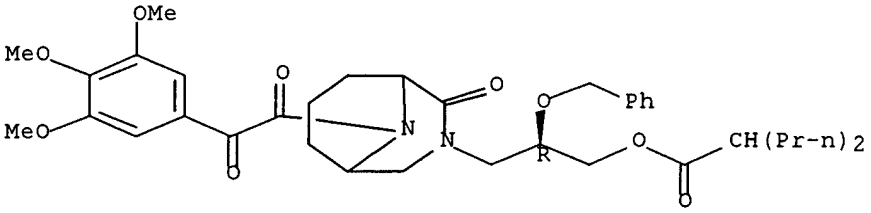
RN 255909-57-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[(2R)-3-hydroxy-2-(phenylmethoxy)propyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



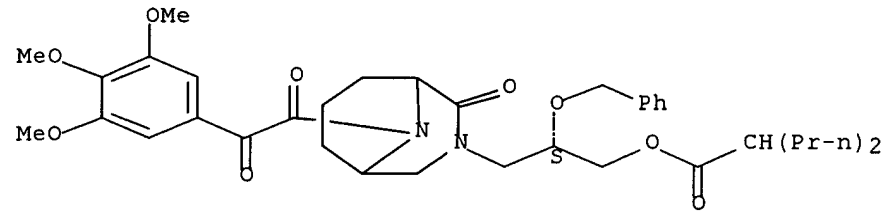
RN 255909-59-2 CAPLUS
CN Pentanoic acid, 2-propyl-, (2R)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



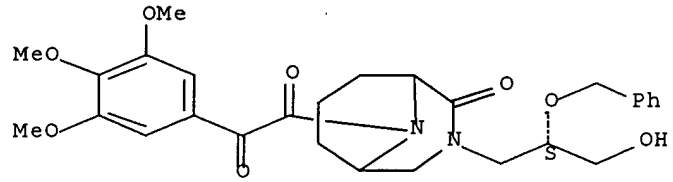
RN 255909-60-5 CAPLUS
CN Pentanoic acid, 2-propyl-, (2S)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

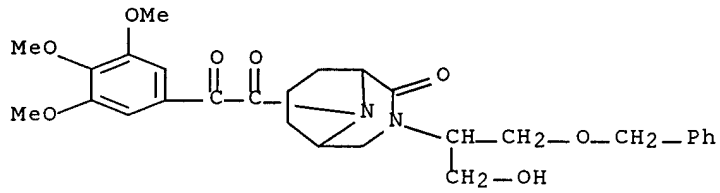


RN 255909-65-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[(2S)-3-hydroxy-2-(phenylmethoxy)propyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

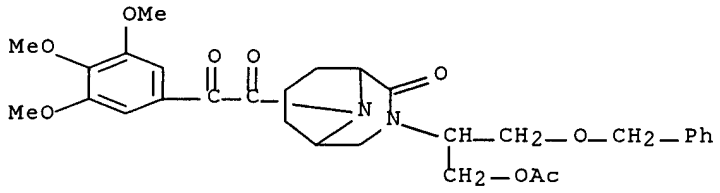
Absolute stereochemistry.



RN 255909-66-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[1-(hydroxymethyl)-2-(phenylmethoxy)ethyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

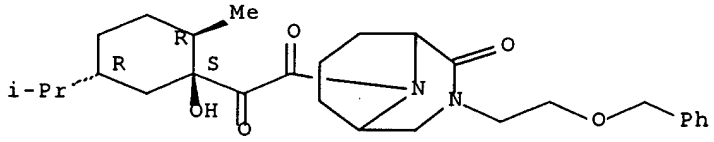


RN 255909-67-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[1-[(acetyloxy)methyl]-2-(phenylmethoxy)ethyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)



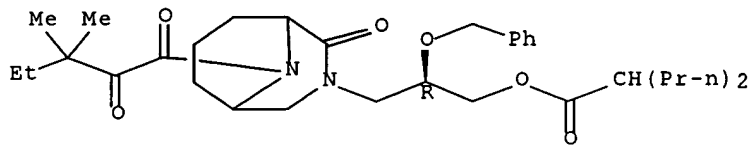
RN 255909-68-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-2-methyl-5-(1-methylethyl)cyclohexyl]oxoacetyl]-3-[2-(phenylmethoxy)ethyl]-, rel- (9CI)
(CA INDEX NAME)

Relative stereochemistry.



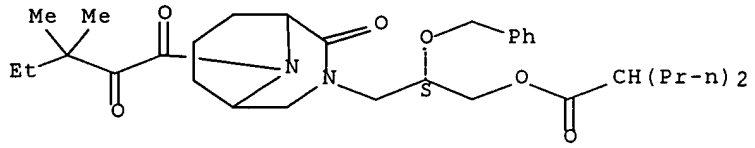
RN 255909-69-4 CAPLUS
CN Pentanoic acid, 2-propyl-, (2R)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



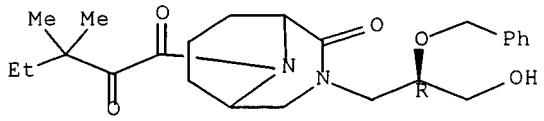
RN 255909-70-7 CAPLUS
CN Pentanoic acid, 2-propyl-, (2S)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



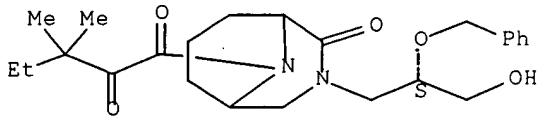
RN 255909-72-9 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-[(2R)-3-hydroxy-2-(phenylmethoxy)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

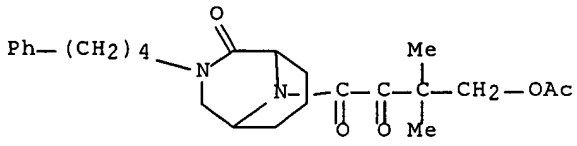


RN 255909-73-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-[(2S)-3-hydroxy-2-(phenylmethoxy)propyl]- (9CI) (CA INDEX NAME)

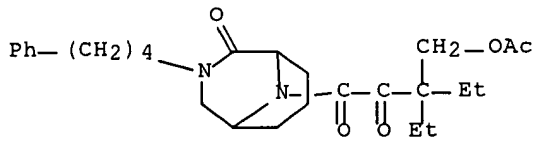
Absolute stereochemistry.



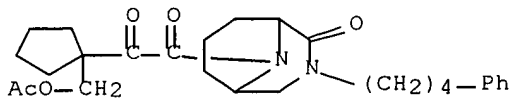
RN 255909-74-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[4-(acetyloxy)-3,3-dimethyl-1,2-dioxobutyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



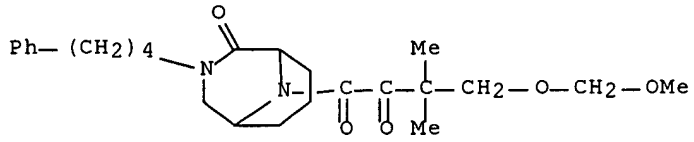
RN 255909-75-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[3-[(acetyloxy)methyl]-3-ethyl-1,2-dioxopentyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



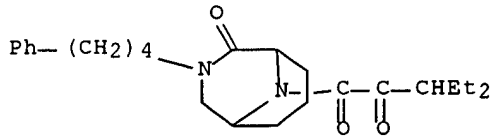
RN 255909-76-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-[(acetyloxy)methyl]cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



RN 255909-77-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[4-(methoxymethoxy)-3,3-dimethyl-1,2-dioxobutyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

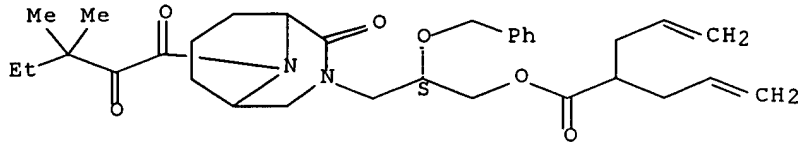


RN 255909-82-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3-ethyl-1,2-dioxopentyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



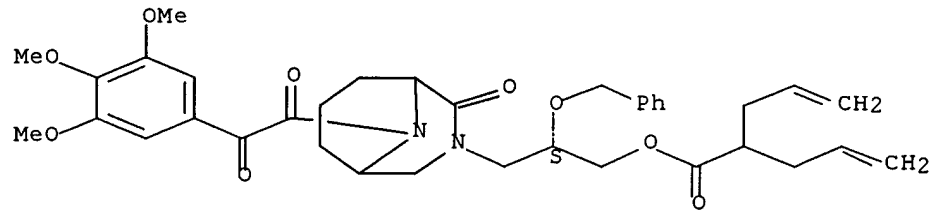
RN 255909-84-3 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



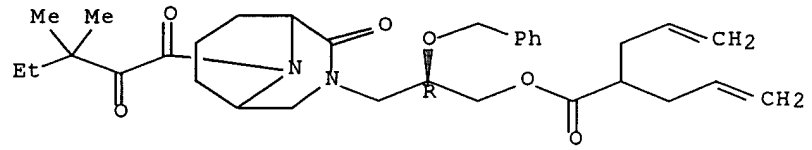
RN 255909-86-5 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



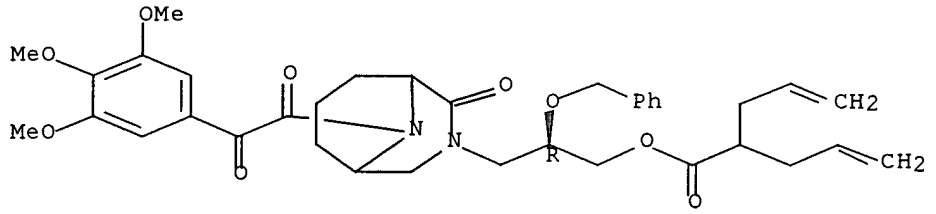
RN 255909-88-7 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

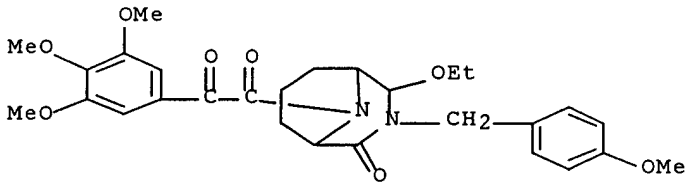


RN 255909-89-8 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

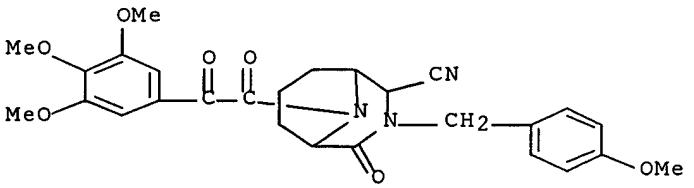
Absolute stereochemistry.



RN 255909-91-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 4-ethoxy-3-[(4-methoxyphenyl)methyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

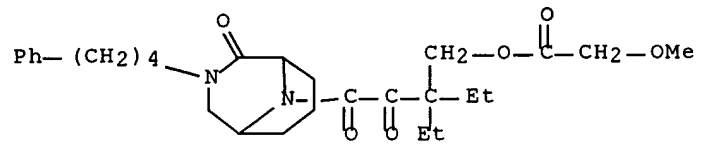


RN 255909-92-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2-carbonitrile, 3-[(4-methoxyphenyl)methyl]-4-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

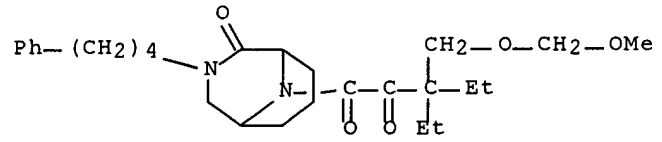


RN 255909-93-4 CAPLUS

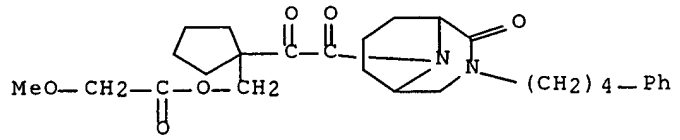
CN Acetic acid, methoxy-, 2,2-diethyl-3,4-dioxo-4-[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]butyl ester (9CI) (CA INDEX NAME)



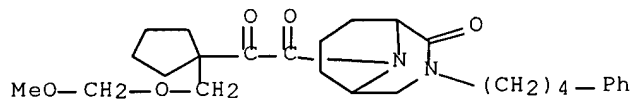
RN 255909-95-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[3-ethyl-3-[(methoxymethoxy)methyl]-1,2-dioxopentyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



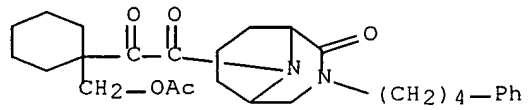
RN 255909-96-7 CAPLUS
CN Acetic acid, methoxy-, [1-[oxo[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]acetyl]cyclopentyl]methyl ester (9CI) (CA INDEX NAME)



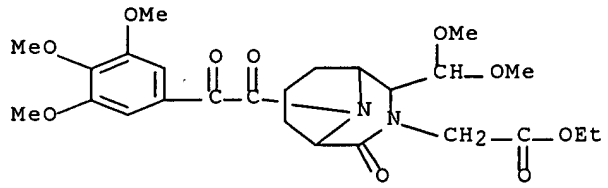
RN 255909-97-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-[(methoxymethoxy)methyl]cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



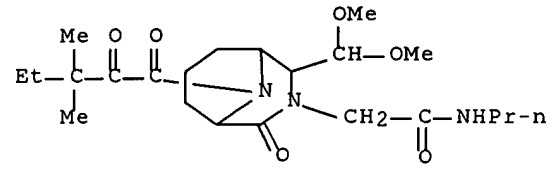
RN 255909-98-9 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-[(acetyloxy)methyl]cyclohexyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



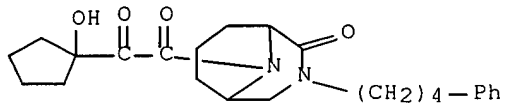
RN 255910-05-5 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-3-acetic acid, 2-(dimethoxymethyl)-4-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



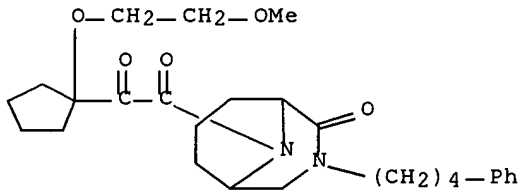
RN 255910-06-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-3-acetamide, 2-(dimethoxymethyl)-9-(3,3-dimethyl-1,2-dioxopentyl)-4-oxo-N-propyl- (9CI) (CA INDEX NAME)



RN 255910-07-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[(1-hydroxycyclopentyl)oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

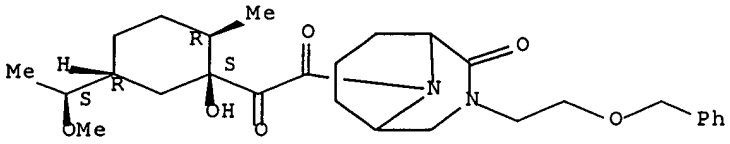


RN 255910-10-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-(2-methoxyethoxy)cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

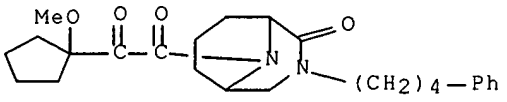


RN 255910-11-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-5-[(1R)-1-methoxyethyl]-2-methylcyclohexyl]oxoacetyl]-3-[2-(phenylmethoxy)ethyl]-, rel- (9CI) (CA INDEX NAME)

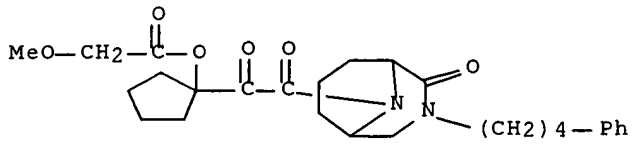
Relative stereochemistry.



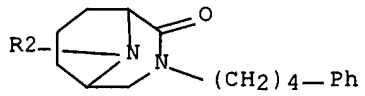
RN 255910-12-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[(1-methoxycyclopentyl)oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

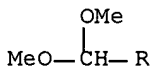


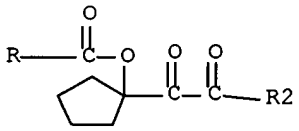
RN 255910-13-5 CAPLUS
CN Acetic acid, methoxy-, 1-[oxo[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]acetyl]cyclopentyl ester (9CI) (CA INDEX NAME)



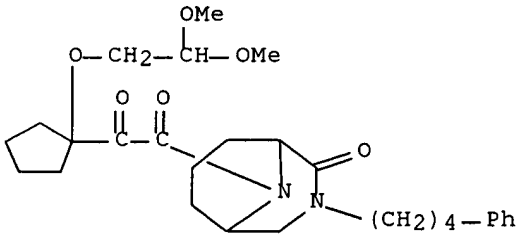
RN 255910-14-6 CAPLUS
CN Acetic acid, dimethoxy-, 1-[oxo[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]acetyl]cyclopentyl ester (9CI) (CA INDEX NAME)





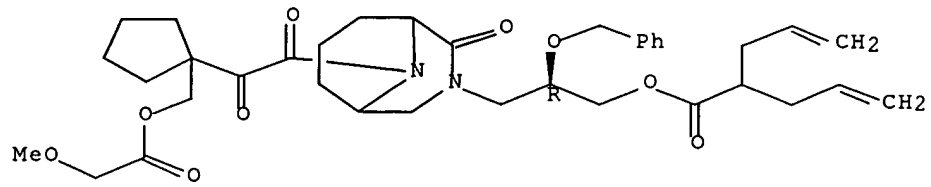


RN 255910-15-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-(2,2-dimethoxyethoxy)cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



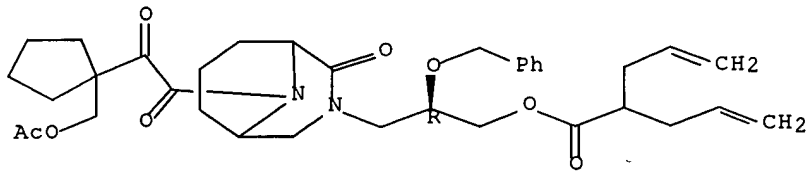
RN 255910-20-4 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[9-[[1-[[(methoxyacetyl)oxy]methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



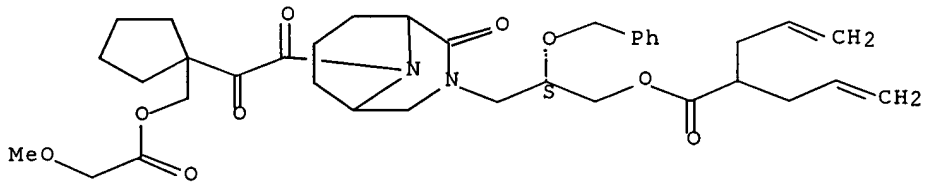
RN 255910-21-5 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[9-[[1-[(acetyloxy)methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



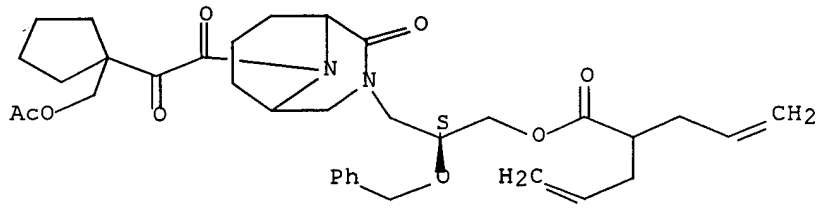
RN 255910-22-6 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[9-[[1-[[(methoxyacetyl)oxy]methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

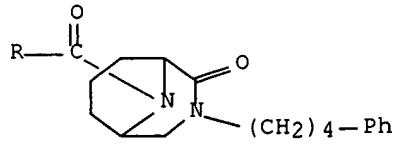


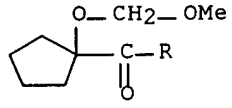
RN 255910-23-7 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[9-[[1-[(acetyloxy)methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 255910-24-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-(methoxymethoxy)cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

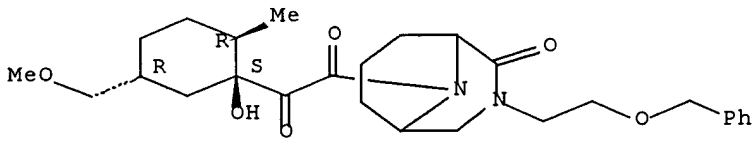




RN 255910-32-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-5-(methoxymethyl)-2-methylcyclohexyl]oxoacetyl]-3-[2-(phenylmethoxy)ethyl]-

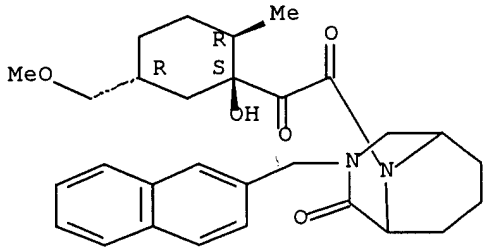
, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

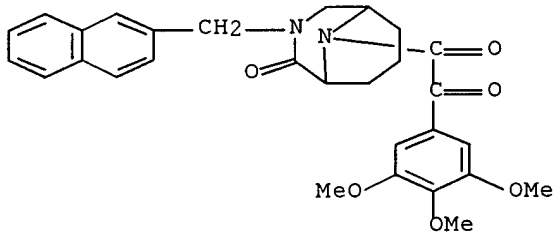


RN 255910-50-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-5-(methoxymethyl)-2-methylcyclohexyl]oxoacetyl]-3-(2-naphthalenylmethyl)-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



RN 255910-51-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-(2-naphthalenylmethyl)-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)



RE.CNT 3
RE
(1) Guilford Pharm Inc; WO 9640633 A 1996 CAPLUS
(2) Guilford Pharm Inc; WO 9716190 A 1997 CAPLUS
(3) Guilford Pharm Inc; WO 9813343 A 1998 CAPLUS

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L1 HAS NO ANSWERS
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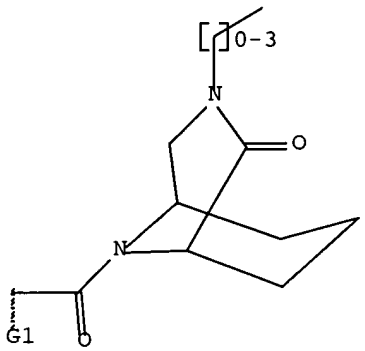

G1 O,X

Structure attributes must be viewed using STN Express query preparation.

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L1 STRUCTURE UPLOADED
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L4 55 S L1 FUL

FILE 'CAPLUS' ENTERED AT 18:06:24 ON 17 APR 2001
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FILE 'MARPAT' ENTERED AT 18:07:26 ON 17 APR 2001
L7 0 S L1
L8 1 S L1 FUL
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	94.62	232.85

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-0.59

STN INTERNATIONAL LOGOFF AT 18:08:32 ON 17 APR 2001

L5 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2001 ACS
AN 2000:68456 CAPLUS
DN 132:107945
TI Preparation of 9-trimethoxyphenyloxalyl-2-oxo-3,9-diaza[3.3.1]nonanes and analogs as FKBP rotamase inhibitors
IN Katoh, Susumu; Kawakami, Hiroshi; Tada, Hiroki; Linton, Maria Angelica; Kalish, Vincent; Tatlock, John Howard; Villafranca, J. Ernest
PA Agouron Pharmaceuticals, Inc., USA
SO PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

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→ 09/356,240 → 7/16/99
60/093,209 7/17/98
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OS MARPAT 132:107945
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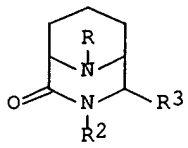


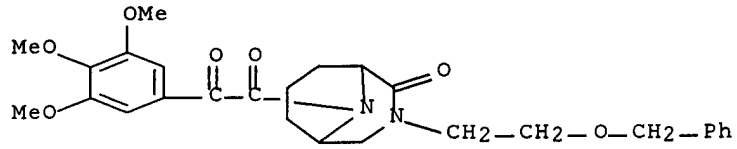
I

AB Title compds. [I; R = COCOR1; R1 = H, (cyclo)alk(en)yl, aryl, etc.; R2 = H, (ar)alkyl, alkoxy(alkyl), alkanoyloxy(alkyl), etc.; R3 = H, cyano, alkoxy, etc.; R2R3 = atoms to complete a ring] were prepd. Thus, piperidine-2,6-dicarboxylic acid was N-protected and the product treated with Ac2O to give the anhydride which was cyclocondensed with PhCH2OCH2CH2NH2 to give, in 3 addnl. steps, I (R2 = CH2CH2OCH2Ph, R3 = H)(II; R = H) which was N-acylated by 3,4,5-(MeO)3C6H2COCO2H to give II [R = COCOC6H2(OMe)3-3,4,5]. Data for biol. activity of I were given.

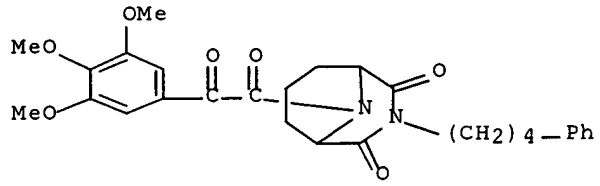
IT **255909-35-4P 255909-38-7P 255909-39-8P**
255909-41-2P 255909-42-3P 255909-43-4P
255909-44-5P 255909-45-6P 255909-46-7P
255909-48-9P 255909-53-6P 255909-57-0P
255909-59-2P 255909-60-5P 255909-65-0P
255909-66-1P 255909-67-2P 255909-68-3P
255909-69-4P 255909-70-7P 255909-72-9P
255909-73-0P 255909-74-1P 255909-75-2P
255909-76-3P 255909-77-4P 255909-82-1P
255909-84-3P 255909-86-5P 255909-88-7P
255909-89-8P 255909-91-2P 255909-92-3P
255909-93-4P 255909-95-6P 255909-96-7P
255909-97-8P 255909-98-9P 255910-05-5P

255910-06-6P 255910-07-7P 255910-10-2P
255910-11-3P 255910-12-4P 255910-13-5P
255910-14-6P 255910-15-7P 255910-20-4P
255910-21-5P 255910-22-6P 255910-23-7P
255910-24-8P 255910-32-8P 255910-50-0P
255910-51-1P 255910-70-4P 255910-71-5P
255910-72-6P 255910-73-7P 255910-74-8P
255910-76-0P
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of 9-trimethoxyphenyloxalyl-2-oxo-3,9-diaza[3.3.1]nonanes and analogs as FKBP rotamase inhibitors)

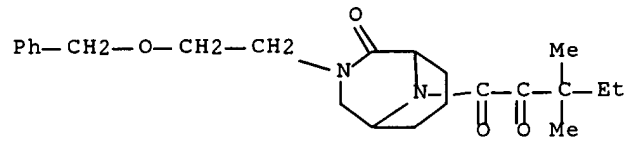
RN 255909-35-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-[2-(phenylmethoxy)ethyl]- (9CI) (CA INDEX NAME)



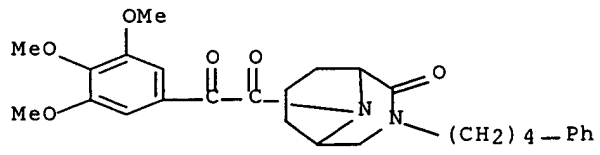
RN 255909-38-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



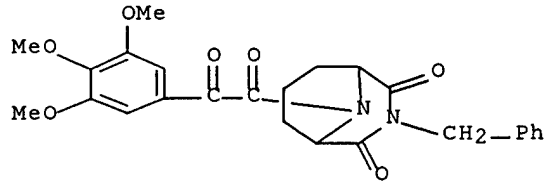
RN 255909-39-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-[2-(phenylmethoxy)ethyl]- (9CI) (CA INDEX NAME)



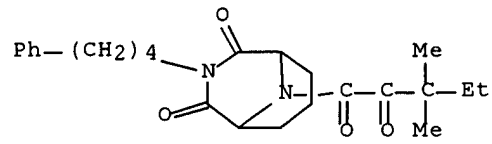
RN 255909-41-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



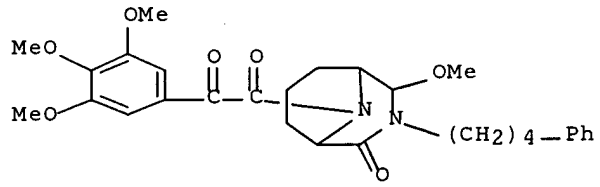
RN 255909-42-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(phenylmethyl)- (9CI) (CA INDEX NAME)



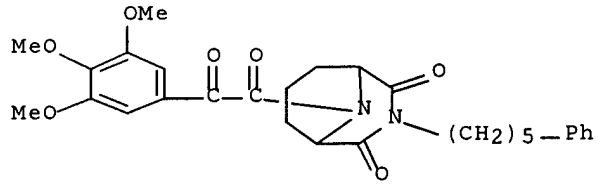
RN 255909-43-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



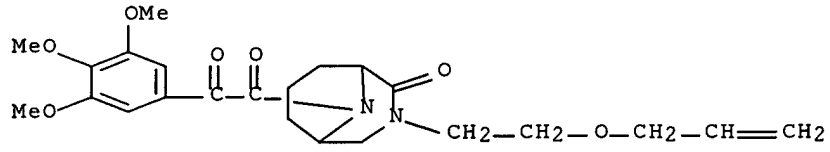
RN 255909-44-5 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 4-methoxy-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



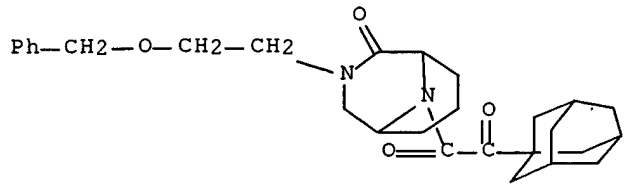
RN 255909-45-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2,4-dione, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(5-phenylpentyl)- (9CI) (CA INDEX NAME)



RN 255909-46-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-[2-(2-propenyloxy)ethyl]- (9CI) (CA INDEX NAME)

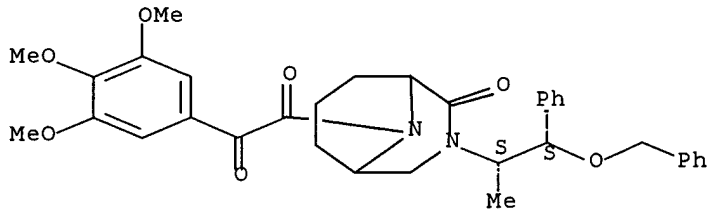


RN 255909-48-9 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(oxotricyclo[3.3.1.13,7]dec-1-ylacetyl)-3-[2-(phenylmethoxy)ethyl]- (9CI) (CA INDEX NAME)



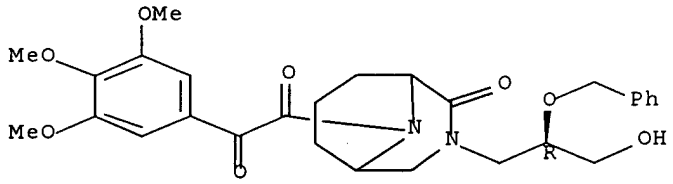
RN 255909-53-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[(1R,2R)-1-methyl-2-phenyl-2-(phenylmethoxy)ethyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.



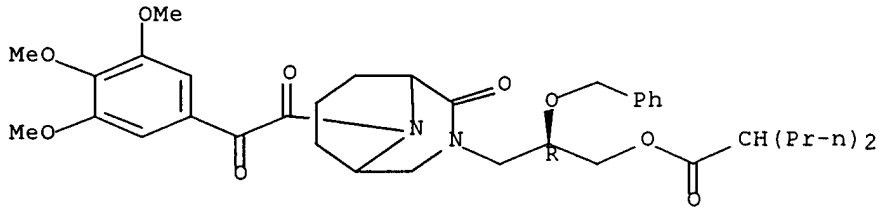
RN 255909-57-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[(2R)-3-hydroxy-2-(phenylmethoxy)propyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



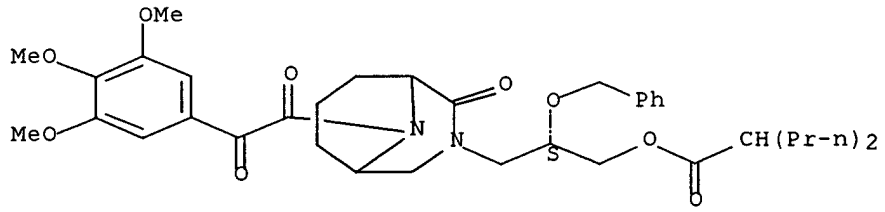
RN 255909-59-2 CAPLUS
CN Pentanoic acid, 2-propyl-, (2R)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



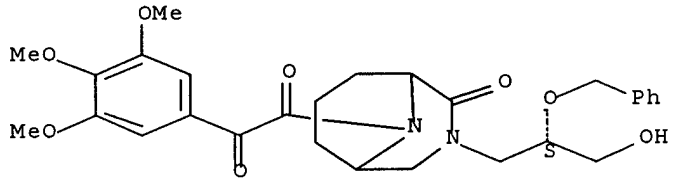
RN 255909-60-5 CAPLUS
CN Pentanoic acid, 2-propyl-, (2S)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

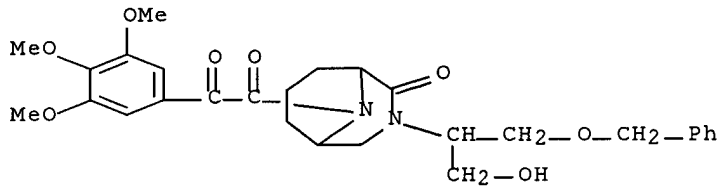


RN 255909-65-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[(2S)-3-hydroxy-2-(phenylmethoxy)propyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

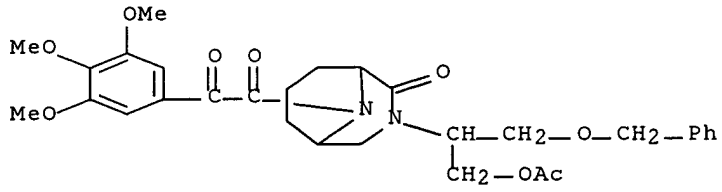
Absolute stereochemistry.



RN 255909-66-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[1-(hydroxymethyl)-2-(phenylmethoxy)ethyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

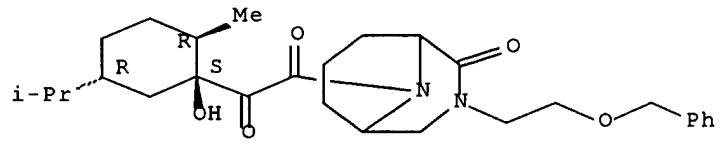


RN 255909-67-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-[1-[(acetyloxy)methyl]-2-(phenylmethoxy)ethyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)



RN 255909-68-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-2-methyl-5-(1-methylethyl)cyclohexyl]oxoacetyl]-3-[2-(phenylmethoxy)ethyl]-, rel- (9CI)(CA INDEX NAME)

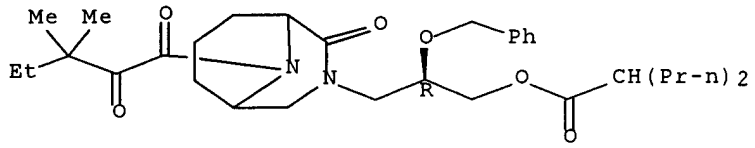
Relative stereochemistry.



RN 255909-69-4 CAPLUS

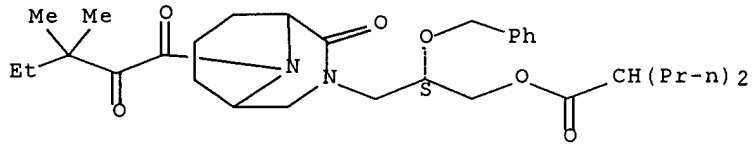
CN Pentanoic acid, 2-propyl-, (2R)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



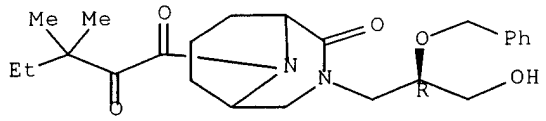
RN 255909-70-7 CAPLUS
CN Pentanoic acid, 2-propyl-, (2S)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



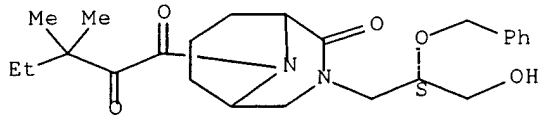
RN 255909-72-9 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-[(2R)-3-hydroxy-2-(phenylmethoxy)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

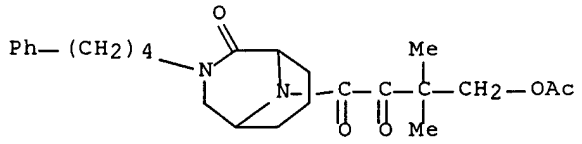


RN 255909-73-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3,3-dimethyl-1,2-dioxopentyl)-3-[(2S)-3-hydroxy-2-(phenylmethoxy)propyl]- (9CI) (CA INDEX NAME)

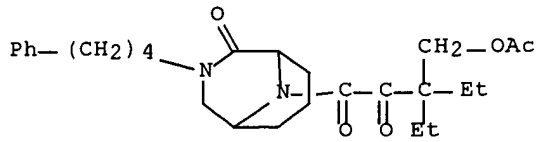
Absolute stereochemistry.



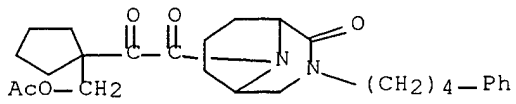
RN 255909-74-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[4-(acetyloxy)-3,3-dimethyl-1,2-dioxobutyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



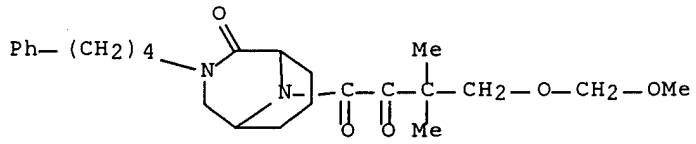
RN 255909-75-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[3-[(acetyloxy)methyl]-3-ethyl-1,2-dioxopentyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



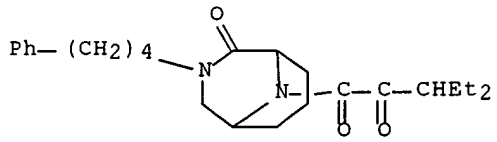
RN 255909-76-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-[(acetyloxy)methyl]cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



RN 255909-77-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[4-(methoxymethoxy)-3,3-dimethyl-1,2-dioxobutyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

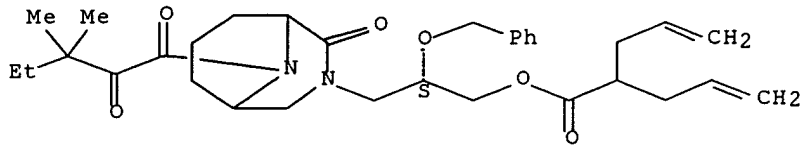


RN 255909-82-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-(3-ethyl-1,2-dioxopentyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



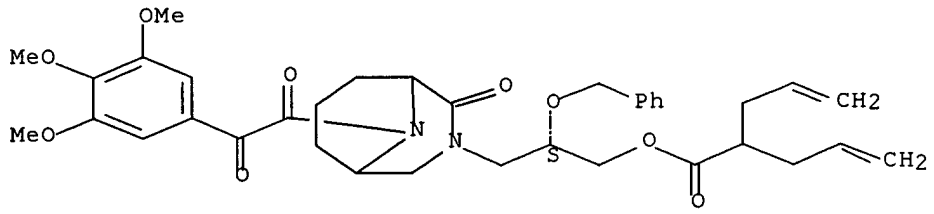
RN 255909-84-3 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



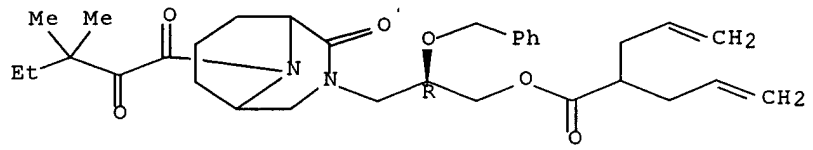
RN 255909-86-5 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



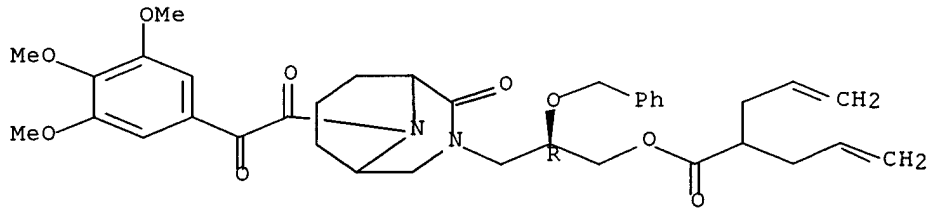
RN 255909-88-7 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[9-(3,3-dimethyl-1,2-dioxopentyl)-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

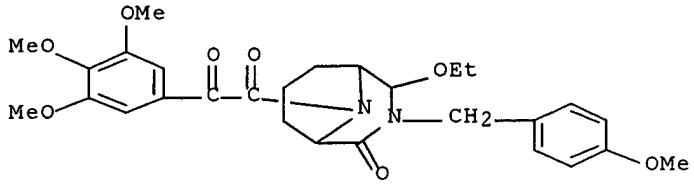


RN 255909-89-8 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[2-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

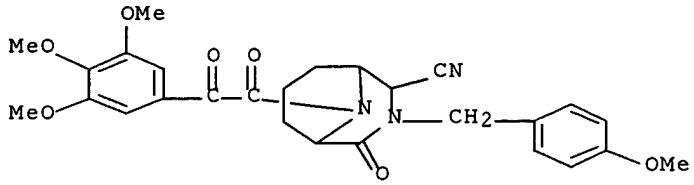
Absolute stereochemistry.



RN 255909-91-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 4-ethoxy-3-[(4-methoxyphenyl)methyl]-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

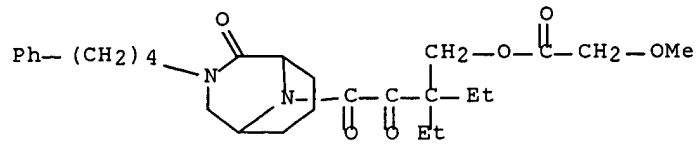


RN 255909-92-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-2-carbonitrile, 3-[(4-methoxyphenyl)methyl]-4-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)

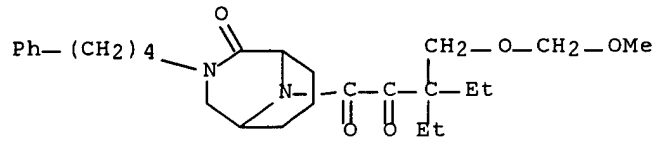


RN 255909-93-4 CAPLUS

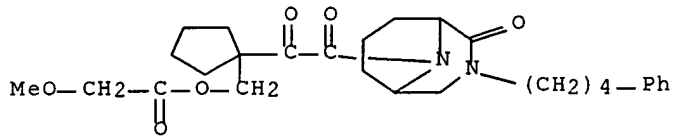
CN Acetic acid, methoxy-, 2,2-diethyl-3,4-dioxo-4-[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]butyl ester (9CI) (CA INDEX NAME)



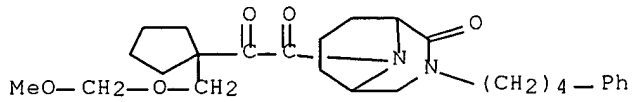
RN 255909-95-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[3-ethyl-3-[(methoxymethoxy)methyl]-1,2-dioxopentyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



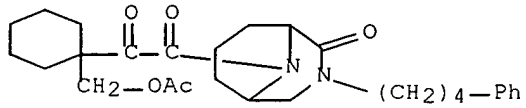
RN 255909-96-7 CAPLUS
CN Acetic acid, methoxy-, [1-[oxo[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]acetyl]cyclopentyl]methyl ester (9CI) (CA INDEX NAME)



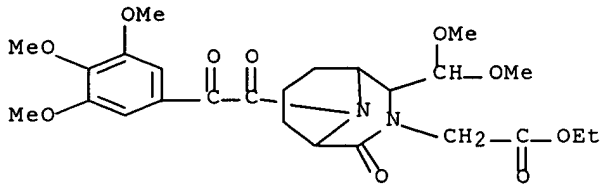
RN 255909-97-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-[(methoxymethoxy)methyl]cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



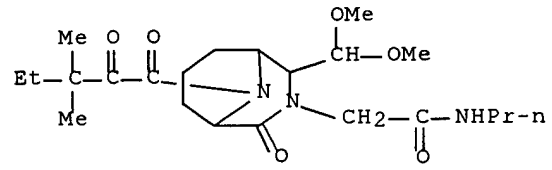
RN 255909-98-9 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-[(acetyloxy)methyl]cyclohexyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



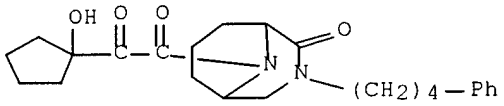
RN 255910-05-5 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-3-acetic acid, 2-(dimethoxymethyl)-4-oxo-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]-, ethyl ester (9CI) (CA INDEX NAME)



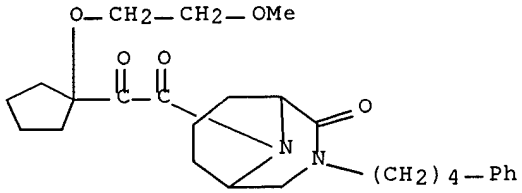
RN 255910-06-6 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonane-3-acetamide, 2-(dimethoxymethyl)-9-(3,3-dimethyl-1,2-dioxopentyl)-4-oxo-N-propyl- (9CI) (CA INDEX NAME)



RN 255910-07-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[(1-hydroxycyclopentyl)oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

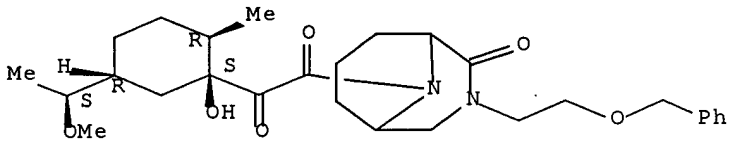


RN 255910-10-2 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-(2-methoxyethoxy)cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

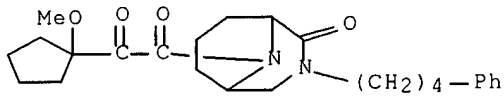


RN 255910-11-3 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-5-[(1R)-1-methoxyethyl]-2-methylcyclohexyl]oxoacetyl]-3-[2-(phenylmethoxy)ethyl]-, rel- (9CI) (CA INDEX NAME)

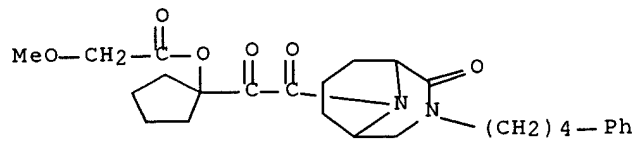
Relative stereochemistry.



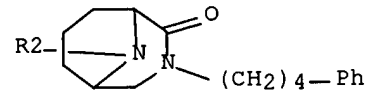
RN 255910-12-4 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[(1-methoxycyclopentyl)oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

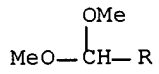


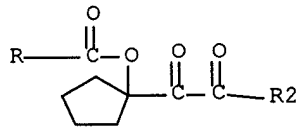
RN 255910-13-5 CAPLUS
CN Acetic acid, methoxy-, 1-[oxo[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]acetyl]cyclopentyl ester (9CI) (CA INDEX NAME)



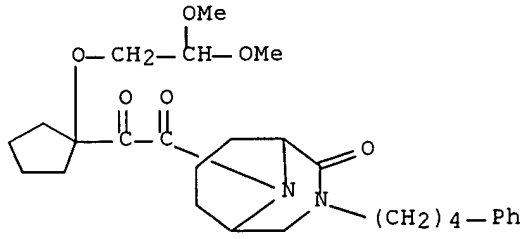
RN 255910-14-6 CAPLUS
CN Acetic acid, dimethoxy-, 1-[oxo[2-oxo-3-(4-phenylbutyl)-3,9-diazabicyclo[3.3.1]non-9-yl]acetyl]cyclopentyl ester (9CI) (CA INDEX NAME)





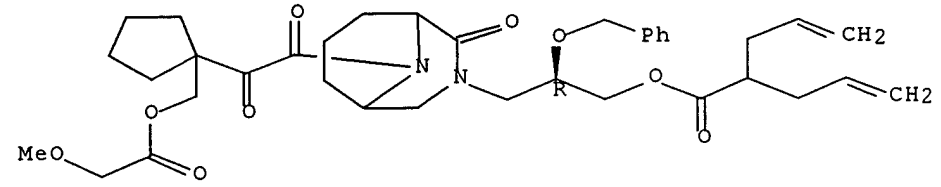


RN 255910-15-7 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-(2,2-dimethoxyethoxy)cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



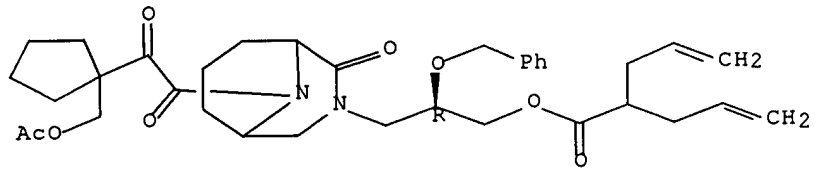
RN 255910-20-4 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[9-[[1-[[(methoxyacetyl)oxy]methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



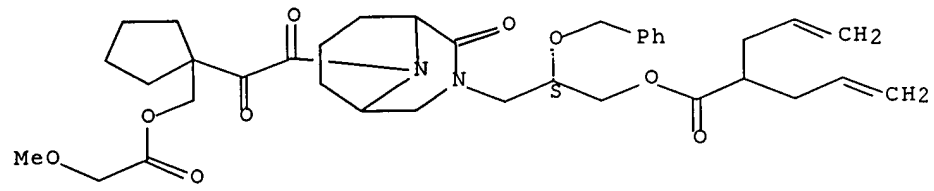
RN 255910-21-5 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2R)-3-[9-[[1-[(acetyloxy)methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



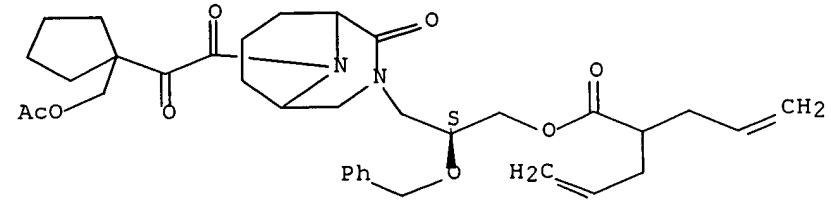
RN 255910-22-6 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[9-[[1-[[(methoxyacetyl)oxy]methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

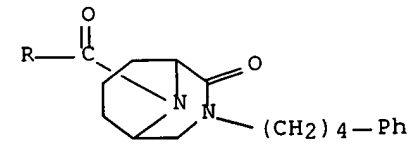


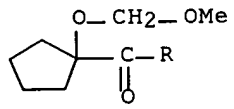
RN 255910-23-7 CAPLUS
CN 4-Pentenoic acid, 2-(2-propenyl)-, (2S)-3-[9-[[1-[(acetyloxy)methyl]cyclopentyl]oxoacetyl]-2-oxo-3,9-diazabicyclo[3.3.1]non-3-yl]-2-(phenylmethoxy)propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



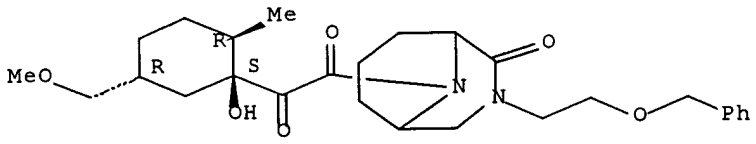
RN 255910-24-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[1-(methoxymethoxy)cyclopentyl]oxoacetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)





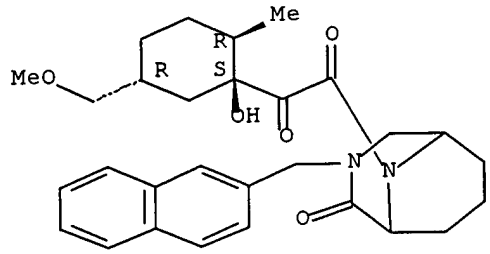
RN 255910-32-8 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-5-(methoxymethyl)-2-methylcyclohexyl]oxoacetyl]-3-[2-(phenylmethoxy)ethyl]-, rel- (9CI) (CA INDEX NAME)

Relative stereochemistry.

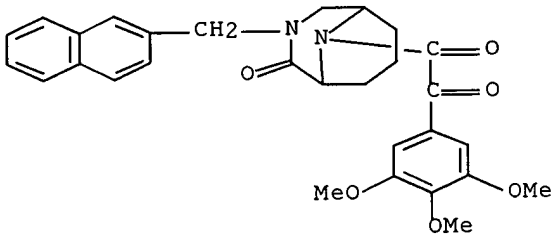


RN 255910-50-0 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 9-[[(1R,2S,5S)-1-hydroxy-5-(methoxymethyl)-2-methylcyclohexyl]oxoacetyl]-3-(2-naphthalenylmethyl)-, rel- (9CI) (CA INDEX NAME)

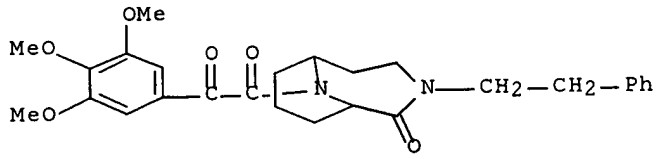
Relative stereochemistry.



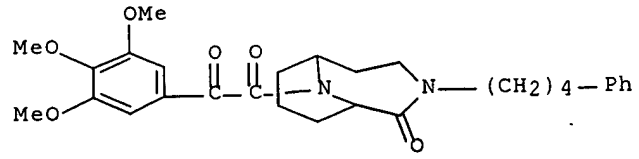
RN 255910-51-1 CAPLUS
CN 3,9-Diazabicyclo[3.3.1]nonan-2-one, 3-(2-naphthalenylmethyl)-9-[oxo(3,4,5-trimethoxyphenyl)acetyl]- (9CI) (CA INDEX NAME)



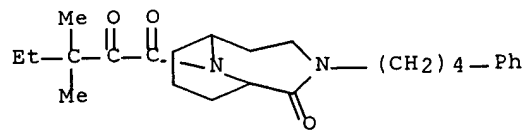
RN 255910-70-4 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(2-phenylethyl)- (9CI) (CA INDEX NAME)



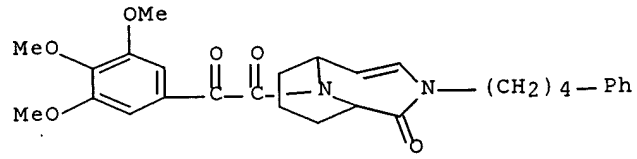
RN 255910-71-5 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



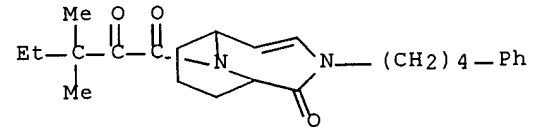
RN 255910-72-6 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-(3,3-dimethyl-1,2-dioxopentyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



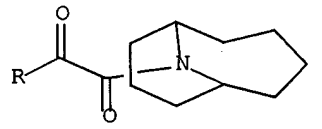
RN 255910-73-7 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]dec-4-en-2-one, 10-[oxo(3,4,5-trimethoxyphenyl)acetyl]-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)

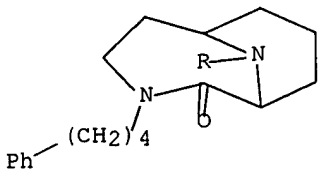


RN 255910-74-8 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]dec-4-en-2-one, 10-(3,3-dimethyl-1,2-dioxopentyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)



RN 255910-76-0 CAPLUS
CN 3,10-Diazabicyclo[4.3.1]decan-2-one, 10-(10-azabicyclo[4.3.1]dec-10-yloxoacetyl)-3-(4-phenylbutyl)- (9CI) (CA INDEX NAME)





RE.CNT 3
RE
(1) Guilford Pharm Inc; WO 9640633 A 1996 CAPLUS
(2) Guilford Pharm Inc; WO 9716190 A 1997 CAPLUS
(3) Guilford Pharm Inc; WO 9813343 A 1998 CAPLUS

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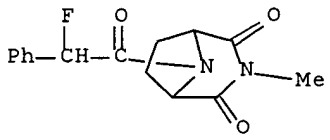
AN 1972:85788 CAPLUS
DN 76:85788
TI Bicyclic homologs of piperazine. XI. 3,8-Diazabicyclo[3.2.1]octane-2,4-diones with potential pharmacological activity
AU Fontanella, L.; Occelli, E.
CS Lab. Ric., Gruppo Lepetit S.p.A., Milan, Italy
SO Farmaco, Ed. Sci. (1972), 27(1), 68-78
CODEN: FRPSAX
DT Journal
LA Italian
GI For diagram(s), see printed CA Issue.
AB The 3-substituted 3,8-diazabicyclo[3.2.1]octane-2,4-diones, I (R = H), are alkylated and acylated and treated with isocyanates to give 3,8-disubstituted compds. I (R = H, R1 = Me) is treated with BuI to give I (R = Bu, R1 = Me). Similarly prepd. are .apprx.30 addnl. I (R = alkyl, acyl, CONH2, CONHPh; R1 = H, Me, PhCH2, aryl). II is treated with NH3 to give I (R = Me, R1 = H); and I (R = H, R1 = p-tolyl) is prepd. by the distn. of III.
IT **35139-96-9**
RL: PROC (Process)
(prepn. of)
RN 35139-96-9 CAPLUS
CN 3,8-Diazabicyclo[3.2.1]octane-2,4-dione, 8-(fluorophenylacetyl)-3-methyl- (9CI) (CA INDEX NAME)



L11 ANSWER 1 OF 1 MARPAT COPYRIGHT 2001 ACS
AN 130:311810 MARPAT
TI Preparation of farnesyl-protein transferase inhibitors
IN Bergman, Jeffrey M.; Dinsmore, Christopher; Graham, Samuel L.
PA Merck & Co., Inc., USA
SO PCT Int. Appl., 138 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9920609	A1	19990429	WO 1998-US21599	19981013
	W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GD, GE, HR, HU, ID, IL, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	AU 9896951	A1	19990510	AU 1998-96951	19981013
	EP 1023270	A1	20000802	EP 1998-951061	19981013
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE, SI, LT, LV, FI, RO				
	US 6103723	A	20000815	US 1998-170951	19981013
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	GB 1998-6432		19980325		
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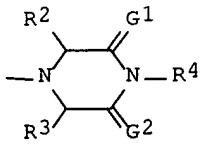
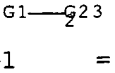
GI



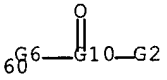
II

AB R1A1Z1A2Z2ZZ4XR [I; A1,A2 = bond, CH:CH, O CO, CONH, etc.; R = e.g., (un)substituted azabicycloalkyl group II; G1,G2 = O or H2; R1 = H, (heteroatom-interrupted) alkyl, heterocyclyl, aryl, etc.; R2R3 = CH2Z3A3(CH2)m; A3 = bond or (hetero)arylene; R4 = alkyl, (hetero)aryl(methyl), -(sulfonyl), etc.; X = bond, CH2, CO, SO0-2; Z = bond or (un)substituted heterocyclylene; Z1,Z2,Z4 = bond or (un)substituted alkylene; Z3 = bond, CH:CH, O CO, CONH, etc.; m = 0-2] were prepd. Thus, prepn. of, e.g., (1R,5S)-3-(3-trifluoromethylphenyl)-8-(4-cyanobenzyl-5-imidazolylmethyl)-3,8-diaza-2-oxobicyclo[3.2.1]octane dihydrochloride was given. Data for biol. activity of I were given.

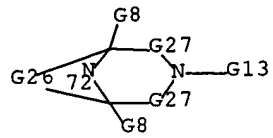
MSTR 1



G1 = 60



G6 = C(O)
G10 = Ak<EC (1-) C, BD (0-) D (0-) T> (SO)
G16 = CH2
G23 = 72

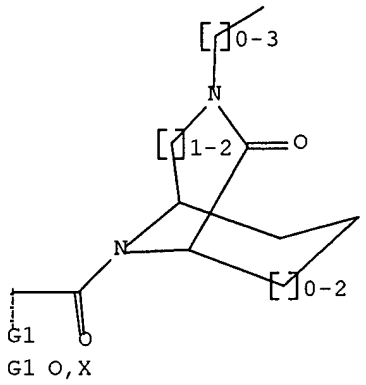


G26 = CH2CH2
G27 = CH2 (SO) / C(O)
DER: or pharmaceutically acceptable salts
MPL: claim 1
NTE: substitution is restricted
NTE: additional ring formation also claimed
NTE: also incorporates claim 2

RE.CNT 1
RE
(1) Occelli; Farmaco Ed Sci 1984, V39(8), P718 CAPLUS

=> d l1; d his; log y

L1 HAS NO ANSWERS
L1 STR



Structure attributes must be viewed using STN Express query preparation.

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FILE 'REGISTRY' ENTERED AT 15:51:30 ON 17 APR 2001
L1 STRUCTURE UPLOADED
L2 QUE L1
L3 3 S L1
L4 62 S L1 FUL

FILE 'CAPLUS' ENTERED AT 15:52:13 ON 17 APR 2001
L5 2 S L4

FILE 'BEILSTEIN' ENTERED AT 15:53:13 ON 17 APR 2001
L6 0 S L1
L7 1 S L1 FUL
L8 0 S L7 NOT L5

FILE 'MARPAT' ENTERED AT 15:53:48 ON 17 APR 2001
L9 0 S L1
L10 2 S L1 FUL
L11 1 S L10 NOT L5

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